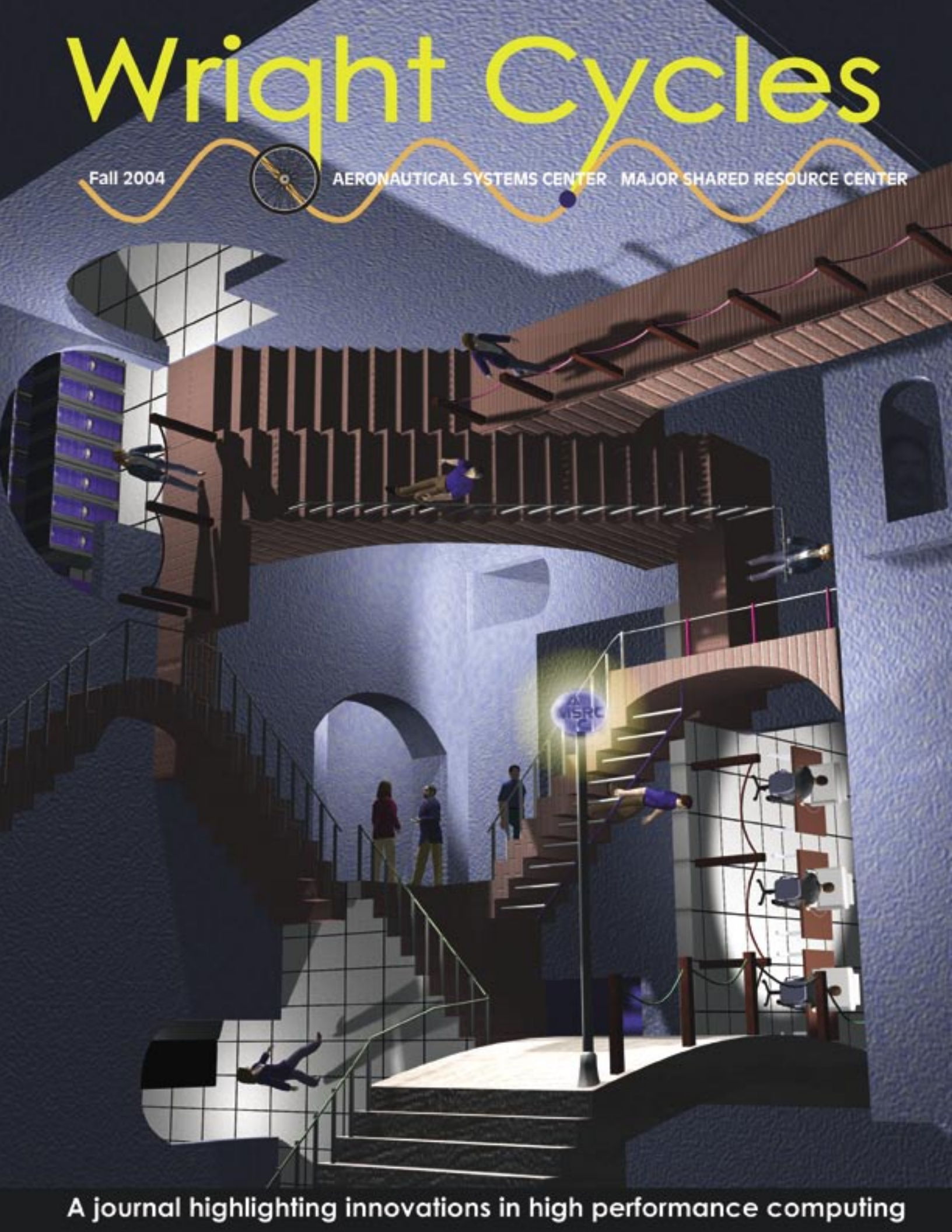
Wright Cycles

Fall 2004 AERONAUTICAL SYSTEMS CENTER MAJOR SHARED RESOURCE CENTER



A journal highlighting innovations in high performance computing

The ASC MSRC Director's Desk

Steve Wourms

"We live in a moment of history where change is so speeded up that we begin to see the present only when it is already disappearing."
-R. D. Laing

My, how the times are changing! We're undergoing a lot of organizational restructuring; we're welcoming new personnel; and HPC systems are undergoing significant changes from multiple aspects.

Our parent organization, the Aeronautical Systems Center (ASC), is performing a massive organizational transformation. ASC is referred to as a "product center" and is charged with the development and acquisition of aeronautical systems, which means that most of the Air Force's aircraft are procured by ASC. Those procurement offices are reorganizing so that they follow the operational Air Force's construct of Wings, Groups, and Flights. As an example, the new structure has a "Long Range Strike Wing," which includes the B-1 and B-2 System Groups, the F-117A and Airborne Electronic Attack System Squadrons, and the J-UCAS System Program Office. This reorg has the added effect of "flattening" the organization from 39 to 23 two-letter organizations. While our "High Performance Computing Division," a.k.a. ASC/HPT, is about to be moved to a two-letter organization, be assured that there will be absolutely no impact to our users nor to our quest to provide premier customer support!

Part of our turmoil is turnover in some key personnel and HPC systems. You can see the full list on Page 22 of this issue of *Wright Cycles*. We're sad to see some key, energetic faces depart; each of them will be very difficult to replace. At the same time we have some real go-getters coming aboard, and they're YOUNG – I don't think they own one 8-track (or 9-track) tape among them!

Finally, the HPC systems. We're looking forward to what's yet to shake out of our Technology Insertion process blender for ASC in FY05. We're confident we'll get a real doozy – a system so big and powerful it'll make your head spin! No, nothing like our friends at Oak Ridge, NASA Ames, or Sandia are installing. And not anything as revolutionary as an "open" or "interactive" system (*See related article on Page 20*). But the systems we're expecting will present us with facility challenges due to their size, weight, and heat output.

Our world is definitely entering a "heyday" for high performance computing. These are exciting times and we plan to make them great times for all of our customers.

The Aeronautical Systems Center (ASC) Major Shared Resource Center (MSRC) is a computational science facility supporting Department of Defense (DoD) research, development, and test and evaluation communities with high performance computing and visualization resources. Created as part of the DoD's High Performance Computing Modernization Program (HPCMP), the ASC MSRC High Performance Computing Center is located on Wright-Patterson Air Force Base (WPAFB) and is one of four DoD MSRC sites. Computer Sciences Corporation (CSC) is the prime support contractor at the ASC MSRC.

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About the Cover: The cover was inspired by SC04's theme *Bridging Communities* and M.C. Escher's 1953 lithograph, *Relativity*. Each scene within the 3-dimensional model has its own Cartesian coordinate system. Arches and steps are used to illustrate collaboration and the aspect of bridging across shared environments.

Approved for Public Release
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ASC 04-1676

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Bridging Communities for the Future

By Jeff Graham, ASC/HPT

Strategic Collaborative Relationships Grow at ASC MSRC

It seems appropriate that the theme of this year's annual Supercomputing Conference (SC04) is "Bridging Communities." Although chosen partly because of the location of this year's conference in the Three Rivers city of Pittsburgh, the theme mirrors some of the exciting activities blossoming at the ASC MSRC. Several emerging strategic collaborative relationships with innovative customers and partners have the center staff excited and energized about the future potential of working with other communities – particularly partners involved in non-traditional high performance computing (HPC) research areas.

The big partnership currently in high gear is a strategic initiative to support the Joint Urban Operations human-in-the-loop (HITL) exercises for the Joint Forces Command (JFCOM) team. A new Linux cluster has been installed at the ASC MSRC, charting a path to deliver a set of technologies that will deliver tremendously powerful modeling and simulation technology to reduce design cycles and enable greater innovation and performance. This new Linux cluster capability is part of a Distributed Center (DC) award by the DoD High Performance Computing Modernization Program Office (HPCMPO). The award has been divided into two systems; the ASC MSRC and Maui HPC Center will be housing and supporting one of these systems. JFCOM Joint Futures Lab team will use the capability to simulate and explore new ways of fighting urban combat. These exercises focus on developing a higher degree of situational awareness in urban environments using sensor technology. The result: the new Linux cluster will increase the fidelity and resolution of exercises, vital to homeland and worldwide security.

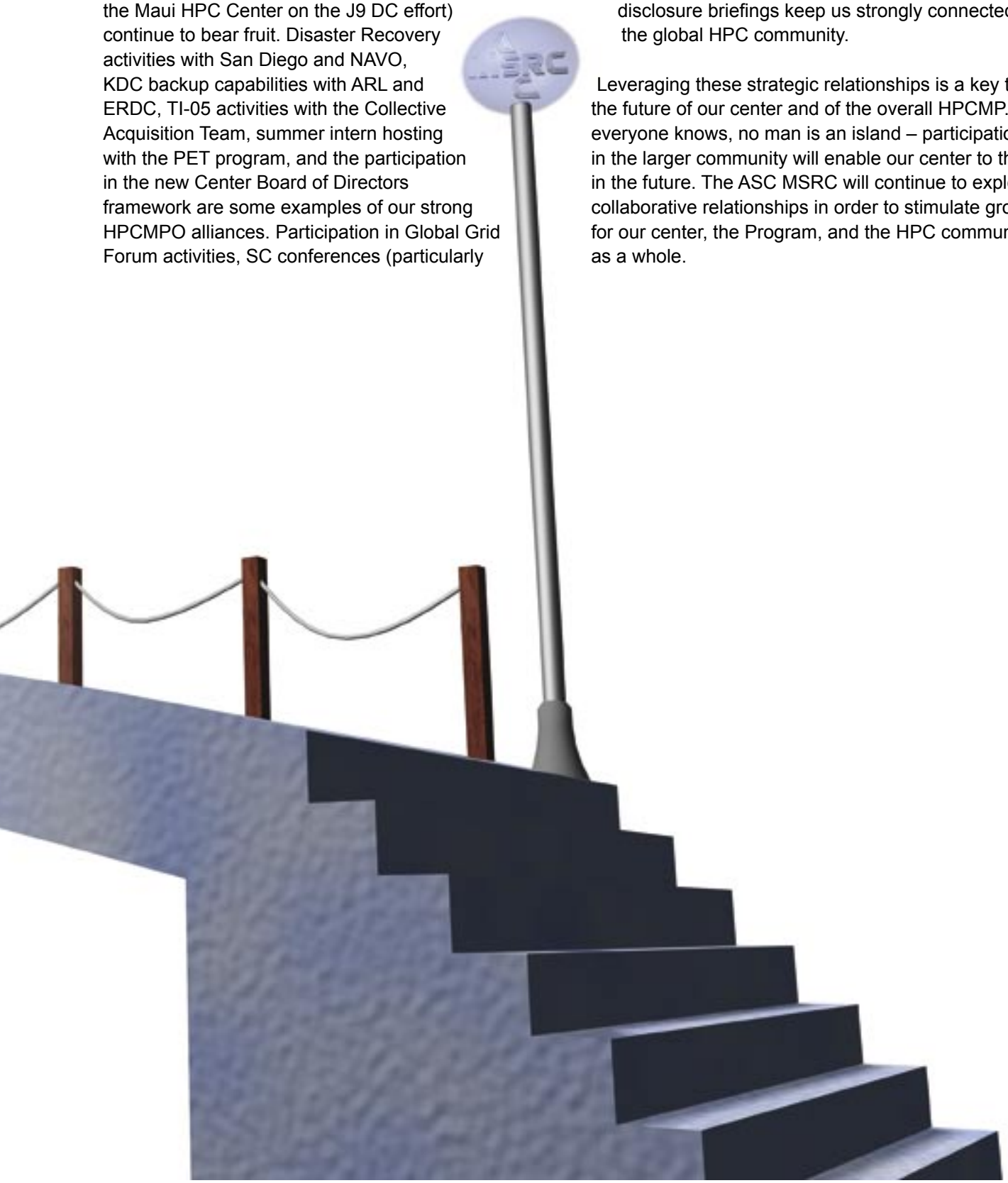
The relationship between the ASC MSRC and the Ohio Supercomputer Center (OSC) dates back to the beginning of the HPCMP through the Programming Environment and Training (PET) activities. Now other opportunities show promise of mutual benefit. OSC is fielding a significant new capability in the new Applied Research and Technology Park in nearby Springfield. OSC will be the second tenant in the park following Lexis Nexis. Plans call for several other major tenants to be announced in the near future. OSC and the ASC MSRC are the key participants in the recently formed Ohio Data Federation, which is pursuing various opportunities that could provide more capabilities for DoD users to leverage HPC resources, specifically in the area of data-intensive computing.

New leadership in the Air Force Research Laboratory (AFRL) – at both the headquarters and the individual directorate levels – has shown an increased interest in leveraging HPC. Discussions with individual directorates include a range of potential projects, ranging from serving data-intensive visualization capability to the user's desktop to hosting directorate level computing resources. An increased focus on the key role modeling and simulation plays in various phases of the acquisition process for weapon systems (including analysis of alternatives and test and evaluation activities) within the Air Force is one reason for the increased demand for HPC resources.

Also, based on our key strategic direction of providing "customer intimate solutions," the ASC MSRC has been actively pursuing a more proactive relationship with several current and potential users. Dr. Alan Wallcraft, through the tireless energy of his S/AAA (Margo Frommeyer) has leveraged our SGI Origin 3000 to the tune of almost 25% of the total FY04 allocations on that system. Discussions with Air Force Weather Agency regarding the reutilization of the IBM P3 could lead to other initiatives to help them more effectively achieve mission goals. The ASC MSRC has worked with Dr. Steven Gorrell of AFRL/PRTF as his research progressed from a pioneer use status with 200,000 hours, to a Challenge Project for FY05 with 3 million hours at the ASC MSRC. The joint efforts between Dr. Gorrell and the ASC MSRC have identified further common areas of interest in the area of data management and storage.

As always, our natural alliances with our sister MSRCs as well as DC activities (working with the Maui HPC Center on the J9 DC effort) continue to bear fruit. Disaster Recovery activities with San Diego and NAVO, KDC backup capabilities with ARL and ERDC, TI-05 activities with the Collective Acquisition Team, summer intern hosting with the PET program, and the participation in the new Center Board of Directors framework are some examples of our strong HPCMPO alliances. Participation in Global Grid Forum activities, SC conferences (particularly our SciNet participation), and frequent technology assessments through HPC resource provider non-disclosure briefings keep us strongly connected to the global HPC community.

Leveraging these strategic relationships is a key to the future of our center and of the overall HPCMP. As everyone knows, no man is an island – participation in the larger community will enable our center to thrive in the future. The ASC MSRC will continue to explore collaborative relationships in order to stimulate growth for our center, the Program, and the HPC community as a whole.



New Infrastructure Capabilities Installed at the ASC MSRC

By Ralph McEldowney, ASC/HPTI

As part of the Technology Insertion 2004 (TI-04) upgrades, the ASC MSRC has added several new infrastructure capabilities in the areas of file servers, mass storage, and networking. Many of these upgrades directly benefit our user community.

The ASC MSRC operates two sets of highly available file servers; one set for user and application home directories, and the other set for mass storage and archival directories. In TI-04, all four of these file servers were replaced. The two new home directory servers are Sun V480s configured with four 1 GHz UltraSparc III processors, 8 GB of memory, and 4 TB of StorageTek D280 disk. The two new mass storage and archival servers are Sun E6800s configured with four 1.2 GHz UltraSparc III processors, 8 GB of memory, and 4 TB of existing StorageTek D178 disk. Both sets of servers replaced machines that were nearly five years old. ASC MSRC users will directly benefit from the upgrade in technology and improved file server performance.

In addition to the file server upgrades, two major changes were made in the mass storage architecture. First, the ASC MSRC upgraded its fibre channel-based storage network by installing two new Cisco MDS 9509 switches. These switches create a fully redundant and managed 2 Gigabit per second (Gbps) storage network. They replaced several smaller switches, which were unmanaged, and operated at only 1 Gbps. All connections between the file servers, attached disk, and storage tapes drives now operate at twice the previous capacity. Second, the ASC MSRC has installed 20 TBytes of SGI TP9500S Serial ATA disk in the storage network. This disk sits between the disk cache on the mass storage file servers and the tape libraries. In other words, this disk acts as an on-line first copy for the most recently accessed user archived data. Users should see a huge improvement in data retrieval times for their most recently accessed files, since it will reside on spinning disks rather than having to be retrieved from tape.

In preparation for the Defense Research and Engineering Network (DREN) access circuit upgrade to OC-48 (2.5 Gbps), the ASC MSRC installed a new Juniper Networks M320 border router. As part of this upgrade, the DREN IP services interface will be upgraded to 10 Gigabit Ethernet (10 Gbps). The Juniper M320 is capable of supporting multiple 10 Gigabit Ethernet modules and higher bandwidth modules in the future. This bandwidth increase will directly benefit the user by increasing the capacity of data that may be moved between DREN sites. While the M320 is the first 10 Gigabit Ethernet capable device in the ASC MSRC network, it won't be the last. A complete 10 Gigabit Ethernet backbone switch will be added in TI-05.

The ASC MSRC continues to enhance its infrastructure to provide a more efficient and effective computing environment for our users. Most of the upgrades implemented in TI-04, such as the file servers, storage network, and network border router, provide a direct performance benefit to our user community. For additional information or to report problems, please contact the ASC MSRC Service Center at 1-888-MSRC-ASC.

ASC MSRC Provides Support to CCM Users at AFRL/ML

By Chuck Abruzzino, CSC

Introduction - by Dr. Ruth Pachter, Senior Scientist, Air Force Research Laboratory, Materials and Manufacturing Directorate (AFRL/ML), and Chief Scientist, ASC MSRC

It is a pleasure to highlight the invaluable support of Drs. Jean Blaudeau, Xiaofeng Duan, and Scott Kajihara to the Computational Chemistry and Materials Science (CCM) user community in AFRL/ML. ML includes the major users of CCM codes at the ASC MSRC.

Theoretical and computational chemistry and materials science is a key area to fulfilling AFRL/ML's mission to plan and execute the Air Force's program for materials and manufacturing in the areas of basic research, exploratory development, advanced development, and industrial preparedness. However, the diversity of materials studied, ranging from polymers and biopolymers, to metal alloys and composites, and electronic materials, require a wide-range of theoretical models, and HPC software, e.g., for quantum mechanical calculations, atomistic simulations, or mesoscale modeling, and continuum mechanics.

The support provided by Xiaofeng, Scott, and Jean, has been important in porting HPC software packages to the center's machines, in providing assistance in aspects of pre- and post-processing, and also in active participation in ML's research projects. Whenever a problem has been identified by a user, a new software package to be run, or an improvement to be carried out, Scott, Xiaofeng, or Jean are ready to help. This has enabled a significant improvement in the utilization of the HPC resources at the ASC MSRC.

Thank you Xiaofeng, Jean, and Scott, for joining our ML community of computational scientists, and helping us use the ASC MSRC resources.

Scott Kajihara has been associated with the ASC MSRC since 1999, originally as a user. He is currently employed by Computer Sciences Corporation (CSC), as a member of the ASC MSRC technical support staff. Scott provides technical support to users of CCM codes and users of the IBM and Compaq HPC systems. He directly supports a variety of CCM codes including the Accelrys software (e.g., Cerius2, CHARMm, Insight II, MS Modeling), MOPAC, and VASP. Over 160 different software packages are installed on the ASC MSRC HPC platforms. As Scott explained, there are a number of utilities that are locally installed and maintained. "Utilities such as editors, visualization tools, and scripting languages really help the users achieve their job with minimum effort," according to Scott.

Xiaofeng Duan is employed by CSC and has served as the application manager for CCM codes at the ASC MSRC since 2001. Before joining CSC, Xiaofeng had been actively running CCM applications at the center since 1996. In addition to installing and maintaining CCM codes, Xiaofeng is responsible for ensuring that the codes are current to the latest released versions and are operational and available. A sampling of codes Xiaofeng directly supports includes ACES II, AMSOL, CRYSTAL, DL Poly, FMD, GAMESS, Gaussian, Gaussview, Jaguar, Jaguar pKa, LAMMPS, MOLPRO, NWChem, Q-Chem, Turbomole, and Wien97. Xiaofeng also supports users by educating them on the use of these applications to fit their research needs. He is also available to troubleshoot any problem they may encounter with the code.

Jean Blaudeau is the CCM PET on-site lead at the ASC MSRC, employed by High Performance Technologies Incorporated (HPTi). HPTi manages

the CCM computational technology area for the entire PET program. HPTi staff work with researchers at AFRL, the Army Research Laboratory, and the Naval Research Laboratory, providing assistance in the use of computational facilities provided through the HPCMP. Additionally, Jean and other HPTi staff are responsible for introducing new technologies to researchers developed by academia. Jean's efforts to initiate meetings between with the 88th Communications Group, the ASC MSRC, and ML led to greatly increased connectivity between the ASC MSRC and ML. "One user mentioned he saw a 90 percent improvement and was very happy with the results," Jean explained.

The other general emphasis of PET requires working closely with the staff in the ASC MSRC User Services. Scott and Xiaofeng are responsible for the installation and maintenance of CCM Codes, and Jean is responsible for the testing of CCM codes. While all three provide support to the user, Jean's role also includes conducting user training. As Jean explained, "We (Scott, Xiaofeng, and I) consistently meet with users to discuss their needs for new chemistry software. We also ensure the codes are installed properly and are used in an optimum fashion on the ASC MSRC HPC platforms."

ML Collaborations

Scott, Xiaofeng, and Jean are also involved in collaborations with ML researchers on CCM projects.

One of the many projects Scott is currently supporting is led by Jeff Simmons of MLLMD. Scott has assisted Jeff in making his phase-field phase-transformation code able to run on different platforms using GNU Autotools, which generate the "configure" generator scripts common in the open-source applications. The technical support team at the ASC MSRC tries to help users get as much execution throughput as possible. In some cases that means helping users with their scripts or system utilities to use the resources more efficiently and get their jobs done.

Xiaofeng is collaborating with Brahim Akdim and Ruth Pachter, MLPJE, on the prediction of properties of single-wall carbon nanotubes. These materials are important for Air Force applications such as light weight composites or cathodes in high-power microwave devices. The characterization of these materials is complex. The insight gained from the theoretical studies, in comparison with experiment, with respect to electronic, optical, and mechanical properties, is important. This research has resulted in several key publications.

Jean has been collaborating with ML researchers for a number of years. One project involves the prediction of ground and excited state properties of platinum containing oligomers; materials that are important for nonlinear optical applications. This work has been in collaboration with the experimental team in MLPJE consisting of Tom Cooper, Dan McLean, Joy Rogers, and Paul Fleitz. In collaboration with Todd Yeates and Doug Dudis, MLBP, Jean has also been studying the electron affinity of C_{122} molecules, which are two C_{60} moieties joined by a C_2 bridge. Understanding the electronic structure of these molecules will help researchers develop novel materials which may have important Air Force applications, such as the development of new conducting polymers or photovoltaic materials. In another project, Jean has been collaborating with Guru Das, MLBP, on the development of the ab initio fragment orbital method, which may enable accurate electronic structure calculations of relatively large molecular systems.

Scott summarized projections for the future as Center staff is looking forward to meeting "the users' requirements for bigger and faster machines" with system upgrades planned in 2005. "We would like to help the user take advantage of running larger jobs on multiple processors."

Verified Materials Modeling and Simulation

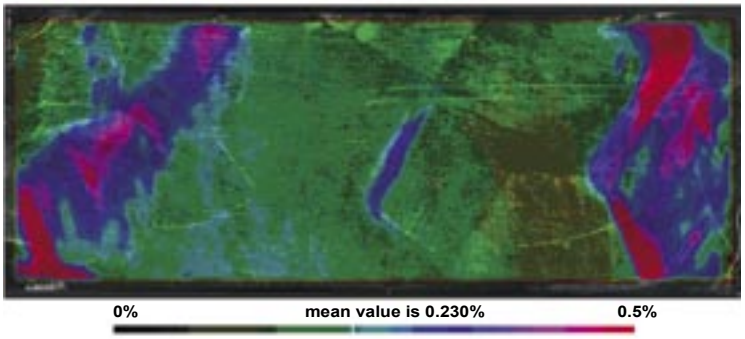
**By David Alan Johnson, Materials and Manufacturing Directorate,
Air Force Research Laboratory (AFRL/MLLMN)**

Full-field measurement techniques have created a revolution in the study of material behavior. Using these techniques, the full two-dimensional or, in some cases, three-dimensional, nonlinear deformation behavior of the surface of a solid can be investigated at a wide variety of scales. At the microstructural level, these techniques enable the evaluation and calibration of modern, sophisticated deformation models to an extent impossible through traditional techniques, such as strain gages. As an example, the localized strain behavior of an advanced intermetallic undergoing mechanical loading is illustrated in the figure. This full-field strain information is available for every loading condition, which enables the study of nonlinear behavior.

It is possible through these techniques to directly study, for the first time, the effect of material directionality of the various microstructural features in polycrystalline engineering materials. In other words, each grain or other microstructure feature may have different material properties in different directions. Studying and modeling this behavior is key to developing a practical, physics-based– design system for the material.

As can be imagined, the amount of data acquired through use of these full-field techniques is very large. Therefore, sophisticated information-management techniques are very important. In addition, the correlation between the full-field experimental results and the results from the modeling and simulation efforts requires the development of new and better tools. Three general areas in which HPC is key to this effort are 1) determination of displacements and strains from raw experimental data, 2) nonlinear modeling of this behavior, and 3) correlation or optimization of the model predictions and the measured physical behavior. Fortunately, all three of these areas involve scalable algorithms and are therefore ideal for an HPC environment.

Efforts are on-going at the ASC MSRC to develop tools for the model/experimental correlation. Sam Naboulsi (CSM on-site, ASC MSRC) has been developing these tools by combining VisualDOC, an optimization software package, and ABAQUS, a finite-element package, to create an automated optimization process to match candidate models with measured material behavior. This automated process will cut model-development time to a small fraction of the time required for traditional material-model development. This, in turn, will lead to much faster insertion of new materials due to the more rapid acquisition of fundamental physical knowledge from this process.



Full-field strain in an advanced-intermetallic specimen.

In addition to the benefits of this effort to the accelerated insertion of new materials, the DARPA Materials Prognosis Program and related programs require that the changes in physical state of a component due to service conditions be completely understood. This is so that field commanders can have complete knowledge of the condition of their vital combat assets. The physics knowledge gained through the true integration of full-field experimental techniques and sophisticated models of material behavior are fundamental to the goals of these important efforts.

Dr. Johnson recently received a Ph.D. from Harvard University.

Contract Year 4 Projects Begin

By Brian Schafer, ASC/HPTT

In June 2004, projects for the PET program were initiated for contract year 4. These one-year tasks support PET's responsibility for gathering and deploying the best ideas, algorithms, and software tools emerging from the national HPC infrastructure into the DoD user community. PET Component 2, hosted at the ASC MSRC, is responsible for the computational technical areas of Forces Modeling and Simulation/C4I (FMS), Integrated Modeling and Test Environments (IMT), and Signal/Image Processing (SIP) as well as the cross-cutting area of Enabling Technologies (ET). A brief description of these projects follows.

SIP
Functional Area POC: Stan Ahalt,
Ohio Supercomputer Center

Mapping Backprojection to the Heterogeneous HPC Cluster for SAR Image Formation

Wide-band, low-frequency Synthetic Aperture Radar (SAR) systems are used by the three services as their principal means of detecting enemy craft on land, air, and sea. A common technique used in image reconstruction is filtered backprojection, where projection measurements from a sensor array are added to all picture elements in an image along the lines of the original projection paths. While backprojection-based processing methods are effective for SAR systems, their high computational complexity has prohibited their use. The goal of this project is to transfer parallelized backprojection techniques from the medical community to the DoD, and speed up SAR image formation an additional 20 times over a single node solution. These parallelized backprojection techniques are targeted to run on the Heterogeneous HPC cluster at Air Force Research Laboratory/ Information Directorate (Rome).

High Productivity Computing (HPdC) for SIP

This project continues efforts from the previous year to transfer new methodologies and software tools that will lead to improved time-to-solution and computational capabilities for the SIP scientists and engineers. This project will port SIP codes and algorithms to high-level, life cycle software tools including MATLAB, P*Matlab, and MatlabMPI. It also investigates next-generation high-end programming environments such as Octave, and delivers a mature version of the web-based interface to MATLAB.

FMS
Functional Area POC: David Pratt,
SAIC

Polygon Decimation Process for Threat/Target Models for Virtual Simulation

The project continues efforts from last year to implement an automated process for taking high fidelity polygonal models of battlefield objects and reducing the polygon count while at the same time maintaining multi-spectral agreement in the visible, IR and radar spectrums. Improvements to this process include enhancements to the evaluation function, using geometric and image metrics to answer the questions "Are they still correlated?"; "Are they simple enough?"; and "Are we done?." Additional IR and radar rendering tools will be investigated for use in the rendering process and 20 examples of threat/target model simplifications will be performed.

IMT
Functional Area POC: Ashok Krishnamurthy,
Ohio Supercomputer Center

Metadata Modeling Using RDF for IMT Data Repositories

In the previous year, a test metadata repository was developed that federated multiple test and evaluation databases that provided a uniform way for test engineers to access test metadata from diverse locations. This project builds upon this repository by creating the necessary framework and software for exchanging and searching the metadata information using the Resource Description Framework (RDF). The goal is to better ensure that as new tests are performed and new databases established (perhaps at new test sites) that this repository can seamlessly integrate new metadata into this common, unified view.

Adapting Parallel Multibody Dynamics Codes

Multibody dynamics software has become an essential tool for developing mechanical systems. Widely used throughout the automotive and aerospace industry, it allows an engineer to create realistic, physics-based virtual prototypes. High fidelity models can take anywhere from a minute to hours, to simulate what occurs in a few seconds in reality. This makes it problematic to fully explore different parameters and

reliability and failure mode analysis, inherently requiring longer run times.

The straightforward way to speed up these codes is to employ parallelism. Unfortunately, there are no commercially available multibody dynamics codes that can take advantage of clusters or shared-memory parallel (SMP) machines. This project will create a converter between LMS DADS, a multibody dynamics package widely used in the DoD, and MBDyn, a free parallelized multibody dynamics code. The converter would enable users to create large, complex models using LMS DADS, run the model on multi-processor system using MBDyn, and then visualize the results with LMS DADS.

ET
Functional Area POC: Robert Moorhead, Mississippi State University

Domain Independent Feature Detection

A set of tools, constructed as separate modules that plug into a common interface that conducts both domain dependent and domain independent feature detection was developed last year. This next twelve-month period focuses on the development of a common interface and language through which the user can interact with the data at the feature level. This feature exploration process provides a common interface and language through which features may be described and through which feature relationships can be determined, thus allowing the user to have a greater understanding of the cause-effect relationship that many of the features have with the underlying geometry and with each other.

Multi-Disciplinary/Multi-Component Data Exchange Specification

In the CFD and CSM disciplines there exists a wide variety of software that supports different sets of data formats. For example, the native grid formats used in grid generation packages such as Gridgen, ICEM, VGRID, Gambit, SolidMesh, ACAD, etc. are different as in the case of flow solvers such as Cobalt, Fluent, Star-CD, OVERFLOW, OVERFLOW-D, and HYB3D, CEA solvers such as XPATCH, and visualization packages like FIELDVIEW, EnSight, Plot3D, and Goggle. This project will develop a toolkit to translate grid and solution data formats across multiple domain applications as well as between different legacy codes.

The toolkit will be provided as a library and can be linked by the legacy codes to read/write the information in the appropriate format. Also, a stand-alone program with a Graphical User Interface (GUI) will be developed which will link to the toolkit library. The GUI can be used to read different types of grid and solution files and convert them into user requested format. This will serve as a demonstration on how to use the data exchange toolkit, as well as to provide the front end for the toolkit.

Mesh Improvement Algorithms and Software Technology

This project concerns the development of methodology, algorithms, and software for constructing improved computational grids and addressing related grid quality issues. A key goal of this project is to transfer enhanced algorithms and software modules for correcting invalid 3D meshes, and improving cell quality. This will increase analysis reliability and project throughput. The proposed work will target unstructured mesh 'failure to complete' and invalid elements from automatic grid generators, anisotropic grids for problems with layers, the development of improved smoothing algorithms and software modules to circumvent the remeshing problem, grid quality metrics, and software implementation to assess local cell quality.

Distributed Design Environment for Solution of Large-Scale Finite Element Models

The fundamental goal of this project is to transfer basic algorithms and data structures necessary to enable effective generalized finite element techniques in a distributed multi-disciplinary modeling environment. This will increase modeling flexibility and capabilities in a number of simulation areas by: 1) exploiting the sophistication of existing analysis packages, 2) promoting efficient management and coherent maintenance of data, 3) making efficient use of the distributed resources, and 4) greatly reducing the architectural impact on the target software. The utility and generality of these techniques will be demonstrated on a highly parallel code, Visual eXtensible Molecular Dynamics (VXMD).

For additional information on current and past activities within the PET Program, please visit the PET Online Knowledge Center (OKC) (*https://okc.erdc.hpc.mil*). The OKC provides access to software tools and products, current information on PET projects, information on past training courses, and the opportunity to register for upcoming training courses. You may also contact Brian Schafer at *Brian.Schafer@wpafb.af.mil*.

PET Welcomes New Staff

By Brian Schafer, ASC/HPTT

In May 2004, the PET Team said good-bye to Ms. Sharron Madero as she moved to a new position as the Office Manager for the new Springfield facility of the Ohio Supercomputer Center. Sharron had been with the PET program for three years, assisting the PET Component 2 Point of Contact (CPOC) in coordinating PET activities, organizing meetings, and preparing reports. Sharron also played a key role in the PET Summer Intern Program, serving as advisor for the interns on security and financial issues, assisting in processing paperwork, helping with travel arrangements to the ASC MSRC, and scheduling final presentations – basically making the intern's experience at the ASC MSRC a successful one!

The PET team was very fortunate to bring Ms. Katherine Rath on board shortly before Sharron left the ASC MSRC. Katherine earned her Bachelor of Arts, and Master of Science degrees at Miami University in Oxford, Ohio. She came to PET from the American Red Cross where she served as a human resource associate. While at the Red Cross, she was responsible for tracking, reporting, and recruiting open positions throughout the organization. Katherine also trained incumbent and new Red Cross employees on corporate policies and procedures.

Prior to her work with the American Red Cross, Katherine was the Assistant Director for MBA Programs for The Ohio State University. Her duties included interpreting university policies and procedures to graduate students and faculty and conducting on-site interviews with candidates at national recruiting forums, conferences, and job fairs. She also served as the primary POC for MBA students navigating college and university policies and assessed applicants for potential admission to the MBA program.

Katherine's business skills and her experience with graduate students helped her adapt quickly before the first summer interns arrived at ASC. We are very pleased to have Katherine on board and wish Sharron all the best in her new position.

Emerging Trends

By Rhonda Vickery, ET on-site lead

This edition of "Emerging Trends" highlights recent progress in the area of remote visualization and gives a preview of some upcoming Enabling Technologies (ET) initiatives.

In the Spring edition of *Wright Cycles*, the basic technical concepts behind remote visualization were described. Since then there has been progress made on several fronts. The first effort conducted by John Vines from ARL, relates to VideoOverIP technology. John has performed some testing to leverage the latest Teraburst Networks V2D product line to collaborate from ARL visualization servers to personnel at other locations. With the right software/hardware combination, this technology has the potential to provide compressed video with remote keyboard and mouse control. For more details, be sure to check out the Fall 2004 edition of the ARL e-Link at *http://www.arl.hpc.mil/outreach* and *http://www.teraburst.com*.

Here at the ASC MSRC, we are in the process of testing the remote visualization capabilities of ParaView in conjunction with the ARL developed Interdisciplinary Computing Environment (ICE). As with any new client-server based software, security testing, and potential enhancements must be considered in order to ensure a capable but secure visualization tool. Since ParaView is open source, there are more alternatives available to make it secure, and several are under active consideration. Developed by Kitware, with funding from the ARL and DOE,

ParaView is an attractive freely available alternative for visualization. For more information on ParaView and ICE, see *http://www.paraview.org* and *http://www.arl.hpc.mil/ice*.

Vizserver is another compressed VideoOverIP solution developed by SGI for remote and collaborative visualization. Version 3.4 is released and is now being evaluated at the ASC MSRC. The server portion runs on SGI high-end visualization systems and distributes interactive sessions to multi-platform desktop client systems. As with any remote visualization solution, network bandwidth plays a major role in how many users can be supported. See *http://www.sgi.com/products/software/vizserver* for more information.

See the ET section of the Online Knowledge Center (*https://okc.erdc.hpc.mil*) for more detailed information on all aspects of remote visualization, tips for using visualization tools on multiple platforms, and reports on the latest technology from relevant graphics related conferences. A new PET ET email newsletter will also begin distribution this fall. Send email to *Rhonda.Vickery@wpafb.af.mil* to be added to the distribution list and to suggest a clever name!

Be sure to check out the other MSRC ET related articles, such as "Visualization Value: Understanding and Developing Smart Materials from First Principles" by Ziegeler, Cooper, and Rappe in the Fall 2004 edition of the Navigator at *http://www.navo.hpc.mil/Navigator*, as well as the latest publication from ERDC at *http://www.erdc.hpc.mil*.

Summer Interns

By Katherine Rath, OSC

In this, the seventh year of the PET Summer Intern program, the ASC MSRC hosted 13 students making it the largest number of students participating in a single year since the program's inception. The internship program provided on-site training for graduate and undergraduate students studying computer science and/or engineering at schools throughout the country. Students participating in the program are given the opportunity to take their classroom knowledge and apply it directly to meaningful projects in a real world environment. At the end of their ten-week appointment, each of the interns gave a final presentation on their accomplishments to ASC MSRC staff and users, which detailed the work that they had done along with the benefits the work would have to the DoD.

During his second year as a PET Summer Intern, James Bittle worked with Rhonda Vickery, Enabling Technologies (ET) on-site lead, on Visualization and Analysis with EnSight, ParaView, and LS-DYNA. James is a senior at Case Western Reserve and is studying Mechanical Engineering.

Robert Culley, of West Chester, Ohio, will return this fall to the University of Cincinnati to finish his Master's of Science degree in Computer Engineering. Upon graduation, he plans to work as a Systems Engineer utilizing his skills in both hardware and software design. During the summer, Robert worked with Paul Sotirelis, the Computational Electronics and Nanoelectronics (CEN) on-site lead, on parallelizing code to compute FDTD results using MPI and reconfigurable computing. He

used the computing resources at both the ASC MSRC and the AFRL/IF DC, to accomplish this task. Robert has interests in reconfigurable design in both hardware and software, and was able to explore the software aspect during his internship.*(See related article on Page 15.)*

Veronica Cornner is a first year Graduate Student working towards a Master's degree in Mechanical Engineering at the University of Alabama in Birmingham. Her undergraduate degree is in Physics. While working this summer with Mason Colbert, PET Training Technologist, Veronica focused on web page development for online training.

Andrew Dragon, from Terre Haute, Indiana, participated in the PET Summer Intern program with the support of his wife Sandy. His plans are to pursue a Master's degree in Aeronautical Engineering after gaining experience in the workforce. With the help of his mentor, Sam Naboulsi, Computational Structural Mechanics (CSM) on-site lead, Andrew researched Foreign Object Damage (FOD) on turbine blades using a finite element analysis approach with the commercial code, ABAQUS. When asked what he thought about the summer internship program, he stated, "I was very thankful for the valuable experience I gained in a professional engineering workplace. Also, I enjoyed the things I learned and the challenge of my project. Sam definitely kept me busy."

Willie Johnson, of Jackson, Mississippi, is a second-year graduate student at Mississippi State University and plans to work in the area of Scientific Visualization (SciVis) after graduation. Rhonda Vickery was his mentor for the summer. Willie's work as a PET Summer Intern involved the visualization of 3D radar data. He used two open-source software packages to produce the visualizations. "I gained exposure to new visualization tools and expanded my knowledge of scientific computing in general," he explained. "I learned a lot that will be beneficial to me in the future."

Michael Lisansky of Tallahassee, Florida, is a senior Industrial Engineering major at Florida State University. As a PET Summer Intern, he worked with Philip Amburn, the Forces Modeling and Simulation (FMS) on-site lead, on a project that included running a constructive model/battle simulator. Michael explained, "What I enjoyed most about being an intern at the ASC MSRC was the exposure to a real world working environment, which is an experience that could not be gained in school."

Steve Molter joined the PET program after receiving his Bachelor's degree in Aerospace Engineering from The Ohio State University. During his internship, Steve worked with Hugh Thornburg, Computational Fluid Dynamics (CFD) on-site lead, performing fluid dynamics analyses on various propulsion applications. His work included a scramjet inlet analysis and a film-cooled vane for a jet engine. According to Steve, "The best thing about working at the ASC MSRC is that there is so much going on here that you are given the freedom to take on as much work as you feel comfortable with." He plans to obtain a Master's degree in Mechanical Engineering and then seek a job in the aerospace industry.

Steven Portal is a senior from Florida International University in Miami, Florida, and hopes to work in the experimental flight area. During his internship, he learned how to conduct experimental research numerically through CFD, while working on three projects; verification and validation of code, grid generation, and post-processing of an Unmanned Air-Vehicle (UAV) and the wing of a Micro Air-Vehicle (MAV). In Steven's words, "Working as a PET Summer Intern was a great experience which gave me an insight to the many different areas of research within the Air Force. My mentor, Hugh Thornburg, helped to broaden my knowledge of CFD, aerodynamics, and the grid generation process."

Alex Schumaker, of Springfield, Ohio, is a recent graduate of The Ohio State University in Aerospace Engineering. He will be pursuing a Ph.D in Aerospace Engineering this fall at the University of Michigan. Alex plans to work as a researcher in hypersonic aerodynamics and air breathing propulsion. During his internship, he worked

with Hugh Thornburg and Dr. Jim Miller, AFRL/VA, on validating the CFD code, AVUS, for use with hypersonic blunt body problems. “Spending the summer with some of the top people in the CFD field has provided me with knowledge and experience that will aid me in my continued education and career.”

James Walker is a senior at North Carolina State University, pursuing a double major in Computer Science and Computer Engineering. He decided to apply for an internship at the ASC MSRC because he felt working with supercomputers, and with people experienced in the field would be valuable work experience for him. “I really enjoyed my time as an intern this summer. I had the privilege to work with very talented people on a real world software project. Plus, I was able to work with combat simulation programs, which were a ton of fun. The hardest challenge I was presented with this summer was the fact that almost everything I had to do was new to me so I first had to learn how to do it. As a result, I learned a lot that I’ll be able to use in the future as a computer scientist, especially if I participate in the program again next summer. I would love to work for the ASC MSRC again. I highly recommend the program to any engineering student looking for a solid internship program.” Philip Amburn served as James’ mentor.

Philip Wheat is a senior at Arizona State University majoring in Aerospace Engineering. Philip worked with Steven Wong, Computational Electromagnetics and Acoustics (CEA) on-site lead, during his internship. His project included working with COBRA code validation to test COBRA’s ability to accurately compute electromagnetic scattering for a number of targets. *(See related article on Page 14.)*

Julian Yarkony of Baltimore, Maryland, is a second-year undergraduate student at The Ohio State University. He plans to eventually work as a professor in Computer Engineering. Julian worked with Jean Blaudeau, Computational Chemistry and Materials Science (CCM) on-site lead, on post processing tools and learned a great deal about C++, software engineering, UNIX, and Python during his internship.

Noah Zier is a senior at Rose-Hulman Institute of Technology in Terre Haute, Indiana. Upon completing his Bachelor’s degree this year in Mechanical Engineering, he hopes to work in the turbine engine industry. Noah worked with his mentor, Sam Naboulsi, on crack propagation in a turbine engine disk using a fracture analysis code called FRANC3D. FRANC3D is a non-commercial code, and thus presented many challenges and obstacles to overcome. At the end of his internship, Noah stated, “This was a great experience for me. I learned many new things through this internship.”

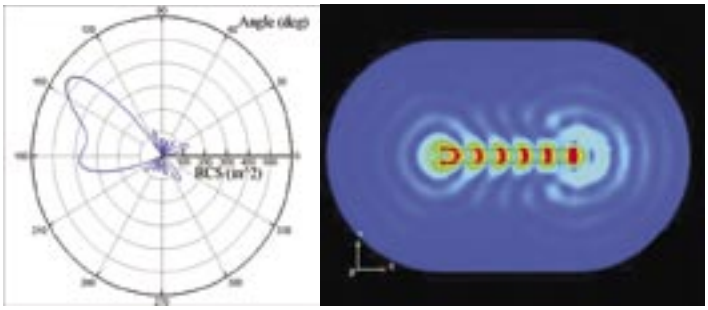
Students interested in pursuing a summer internship in 2005 should contact Katherine Rath at *katherine.rath@wpafb.af.mil* or Bill Zilliox at *william.zilliox@wpafb.af.mil.*

COBRA Electromagnetics Solver Testing at the ASC MSRC

By Steve Wong, CEA on-site lead
José Camberos, AFRL/VAAC

Researchers at the Computational Sciences Center, AFRL/VAAC, have been engaged in the development of a parallel finite–volume time–domain computational electromagnetics (CEM) solver for the past few years. The current version of the solver, COBRA, traces its lineage to Cobalt60, a CFD code also successfully developed at AFRL/VAAC. COBRA uses unstructured 3D meshes that offer greater geometric modeling flexibility than algorithms such as the finite–difference time–domain (FDTD) for solving Maxwell's equations. In addition, the same geometric mesh can be shared by both COBRA and Cobalt, which makes possible more efficient couplings when tackling multi–physics problems involving CEM and CFD. After initial development, COBRA has now reached the stage where it is ready for systematic Verification and Validation (V&V). In collaboration with the PET Program, the COBRA solver was put through a battery of tests on the SGI Origin 3900 at ASC MSRC, one step in the V&V process of this code.

José Camberos (AFRL/VAAC) teamed up with Steve Wong (PET CEA on-site lead at ASC MSRC) and identified a COBRA V&V project for PET Summer Intern student Philip Wheat, a college senior in Aerospace Engineering at Arizona State University. Since numerical accuracy is a key element of the CEM solver, the goal of this project was to test COBRA's ability to accurately compute electromagnetic scattering for a number of targets. The targets chosen include the Electromagnetic Code Consortium (EMCC) Open Pipe benchmark, the X-43 Hypersonic Aircraft and the X-45 Unmanned Combat Air Vehicle (UCAV). Monostatic and bistatic radar cross sections (RCS) were calculated at various frequencies for the Open Pipe benchmark. The results obtained by COBRA matched very well with the experimental data published by the EMCC and will be submitted to the EMCC for further validation. An example of the scattering pattern and bistatic RCS is shown in Figure 1. In addition to the canonical Open Pipe benchmark, Mr. Wheat also performed tests on the X–43 Baseline Hypersonic Vehicle and the X–45 to support ongoing activities at the AFRL Air Vehicles Directorate. An example of the electromagnetic scattering pattern for the X–43 is shown in Figure 2.



(a) (b)

Figure 1. Example of bistatic RCS pattern (a) and corresponding scattered electric field (b) for the Open Pipe Geometry with incident wave oriented 15° from centerline.

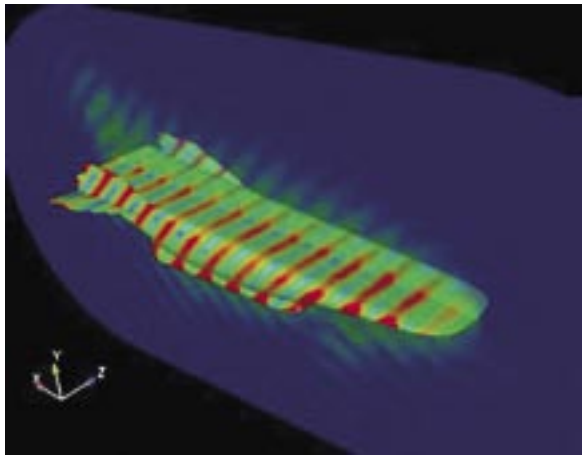


Figure 2. Electromagnetic Scattering (contours of scattered E-field magnitude) from X-43 Hypersonic Vehicle. Incident wave oriented 45° from underside.

This kind of collaboration between the PET Summer Intern program and DoD research labs, as exemplified by this project, has been very beneficial to both the students and researchers involved. As a testament of what can be achieved in a short period of time by an enthusiastic and intelligent student, in just ten weeks, Mr. Wheat made a solid and practical contribution to ongoing research at AFRL/VAAC. In appreciation of his work and in recognition for a job well done, an AFRL Junior Researcher Award was presented to Mr. Wheat at the end of his summer internship by Dr. Camberos.

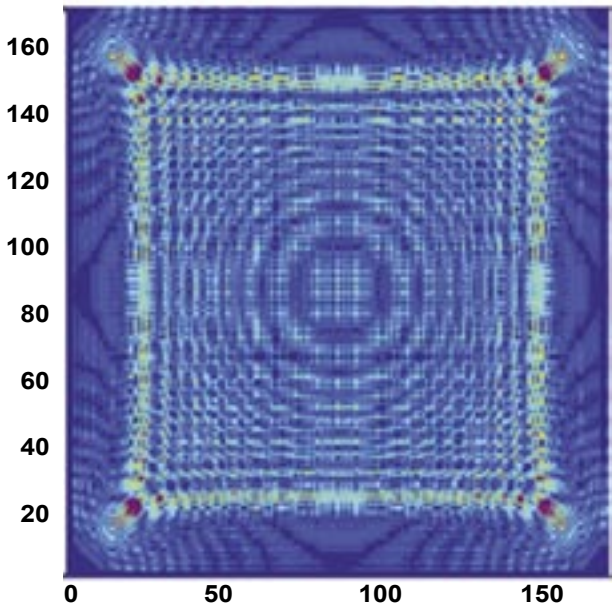
Additional information on the COBRA EM solver can be obtained by contacting Dr. José Camberos (AFRL/VAAC) at *Jose.Camberos@wpafb.af.mil*.

Summer Internship: A First Hand Account

By Robert Culley

Robert Culley is pursuing a Master's degree in Computer Engineering at the University of Cincinnati. During the summer of 2004, he participated in the PET Summer Intern Program at the ASC MSRC. While at the ASC MSRC, Paul Sotirelis, Computational Electronics and Nanoelectronics (CEN) on-site lead, served as his mentor. Following is Robert's account of his summer internship experience.

I began my PET summer internship at the ASC MSRC with some apprehension, but the staff at the ASC MSRC made me feel welcome and started getting me set up for my ten weeks of work. By the end of the week, I felt quite at home. The base seemed more a community than what I thought an Air Force Base would be like. I spent most of my time working on the project that my mentor and I had agreed upon. I also had the opportunity to go on tours of different base facilities; the most interesting of which was a tour of the ASC MSRC HPC floor, which contains equipment that my fellow interns and I were using to complete our tasks.



The z-component of the electric field corresponding to a progagating electromagnetic pulse is shown for a two-dimensional rectangular waveguide.

As part of my project, a two-dimensional finite-difference time-domain (FDTD) MPI code that made use of a two-dimensional domain decomposition topology was created. I used code contributed by others involved in the CEN-04-006 PET project as a starting point. Additionally, a detailed analysis of the code's scalability on the ASC MSRC systems was performed. Since a key goal of my project was to run this code on reconfigurable hardware, I examined decompositions where the local data size was fixed in addition to the more usual fixed global data size decompositions.

Toward the end of my internship, I focused on modifying the code for use on reconfigurable hardware. The target system was the AFRL/IF Hetereogeneous HPC (HHPC). This machine uses both CPUs and field programmable gate arrays (FPGA), with a pair of FPGAs on each of the 48 nodes. As part of this focus, I attended a workshop in Rome, New York and heard how other people were using the HHPC. I returned from the trip excited about the prospects of running some code on that system, but my time ran out before a performance analysis could be completed on this system.

During the internship, I encountered many challenges, some of which were my own creation. However, I worked through these challenges and the final results even had a symmetrical beauty when plotted in MATLAB. I look back on my internship with a sense of accomplishment and an excitement for HPC, which I hope to continue as a Master's student in Computer Engineering at the University of Cincinnati.

User Tips

By Tracey Smith, CSC

The Customer Assistance and Technology Center (CATC) staff is committed to providing premier customer support to our users. As part of that commitment, members of the CATC staff are providing a set of tips to help users to navigate the ins and outs of our computing environment. Additional tips and answers to frequently asked questions can be found on our web site at *www.asc.hpc.mil*.

Visual Queue

In the last issue of *Wright Cycles* we introduced Visual Queue, the web-based application that lets you visually monitor the life cycle of jobs in the queues at the ASC MSRC. Now it's time to show you how to access and operate the Visual Queue.

Visual Queue is accessible from the ASC MSRC web site. Once you are on the site you click on the login button at the top right hand corner. This will take you to a page where you must log in using your Kerberos user name, password, and secure-ID passcode. You are next directed to a page that allows you to access Visual Queue or change your password. After you click on Visual Queue you are given some basic instructions and several options. You can view the queues live, or replay past activity. You can also choose to see the Compaq complex, the Origin 3900, or both on a single page. A new feature also allows you to view a chart of the number of jobs queued and the system load for periods up to the last 90 days. If you select to view the queue, you will be presented a display that has the name of the system at the top, a depiction of the queue on the left, and a representation of the system on the right. A box at the bottom right gives the system utilization.

In the queue, individual jobs are represented by circles. The size of the circle and the number in the circle represent the number of processors requested. The color of the circle shows how long the job has been waiting. Left clicking on a circle will give you more information about the job including job ID, user ID, the requested run time, the current wait time, and the number of additional jobs that this user has running or waiting.

On the system display the small boxes represent individual processors on the system and the colors represent the status of the processors. White processors are idle, while running jobs are shown as various shades of blue. The darker the shade of blue, the closer the job is to completing. Left clicking on a processor will give additional information about the job including the job ID, the user ID, the number of processors, the requested run time, the run time remaining, and the number of jobs this user has running or waiting.

Data Conversion for Different Platforms

One of the common problems that arise in a multiple platform environment like the ASC MSRC, is the capability to use binary data files generated on one system, on another system. For example, a user may want to use visualization tools on the Scientific Visualization Lab SGI machines to render data generated on the Compaq SC-40/45 complex. If the user used the data as-is, they would get erroneous results.

The issue is that the ordering of data is different on the SGI and Compaq machines. Since most scientific data consists of multi-byte storage elements (typically four or eight bytes to store a number), the ordering of those bytes is significant. A choice is made to store either the byte with the leftmost (highest order) bits or the rightmost (lowest order) bits first in memory. The former is referred to as big-endian, and the latter as little-endian. SGI machines store data in big-endian format; Compaq machines in little-endian format.

To convert between big-endian and little-endian formats use the command:

```
dd conv=swab if=input-file of=output-file
```

The dd(1) command is available on all Unix systems.

Finding Your Disk Usage

Use the ***quotachk*** command to find out how much space you are using. This command grabs your disk usage from a flat file that is generated every 10 minutes by a system cron job. ***quotachk*** will give you the most reliable count of your usage; however, you must be aware of the update schedule since recent changes will not appear in the number until the next

scheduled update.

Disk quotas are enforced only on the user's HOME directory. The default limit is currently set to 512 Mbytes. There are no disk quotas on /workspace or the archive directories.

qprep

The primary queuing system in use at the ASC MSRC is the Load Sharing Facility (LSF), but we also support the qprep batch scripting language that has been developed as part of the Practical Supercomputing Toolkit (*http://pstoolkit.org*). ***qprep*** allows a user to write one script that can be submitted to any of our systems with little or no modification and also can be run at any other site that supports qprep. ***qprep*** converts the qprep script to that system's native batch scheduler language and, optionally, submits it for the user. The syntax for ***qprep*** is;

qprep [key1=value1[key2=value2 ...]] filename

For users to easily generate a basic qprep standard script without any qprep knowledge, a tool called "***gen-qprep***" is provided by the ASC MSRC. To use the tool to generate a new script, a user just needs to issue a command:

gen-qprep -f script_name

and then follow prompts to answer the questions regarding number of processors, walltime, queue name, etc.. The queuing settings will be included in the script in qprep standard. One can add his/her own commands after the qprep settings in the script and use command:

qprep script_name

to translate and optionally to submit a batch job into the queue on the current machine.

Moving Data to the ASC MSRC

One of the problems users encounter in getting started using the ASC MSRC is how to transfer their data to our environment. Due to security restrictions, the transfer of data is not always straight forward. However, there are three good tools available. Each is described below.

- **File transfer protocol** (***ftp***) is the most familiar transfer mechanism and is used to transfer files with sizes typically ranging from Kbytes to several Mbytes. We use an encrypted ftp program to transfer files. Users will need to download a copy of the encrypted ftp program and install it on their local system in order to use ftp files to the ASC MSRC. The software is part of the Kerberos distribution.
- **Secure copy** (***scp***) can also be used to copy files to and from our systems. The contents of the file are encrypted for secure transfer of information. Since there is some overhead associated with encryption, the transfer rate you experience may be slower than with ***ftp***. The file size typically would range from Kbytes to several Mbytes.
- **Multiple-path secure copy** (***mpscp***) should be used to copy very large files between ASC MSRC systems. ***mpscp*** uses multiple transmission control protocol (TCP) streams (and multiple network interface cards, if available) to segment a large file into pieces and send the pieces in parallel, reassembling them into a single file on the remote side. The user will need to contact the ASC MSRC Service Center for information on how to obtain client kits.

For more information see the ***man*** pages on any machine at the ASC MSRC.

Xcygwin

ASC MSRC users who connect to the center using Windows based PCs have traditionally been at a disadvantage because their systems do not support the display of graphical data from UNIX Xwindows. The only solution for this was to purchase a commercial Xserver. In order to solve this problem, the ASC MSRC has created a packaged version of the XFree86 Xserver that is available in the Cygwin software package. This package is designed for users who wish to have remote X capabilities, but do not wish to install the full Cygwin package or pay for a commercial Xserver. As such, it is designed for users who DO NOT have Cygwin currently installed. If you have Cygwin installed, please use the Cygwin setup program provided with it to obtain the XFree86 package as installing the ASC MSRC packaged Xserver can corrupt your current Cygwin install.

Contact the ASC MSRC Customer Assistance and Technology Center via email at *msrchelp@asc.hpc.mil* or 1-888-677-2272 if we can assist you in any way.

3D Structure of Pitched-based Carbon Foams

By Benji Maruyama, AFRL/ML

Pitch-based carbon foams are a new class of multi-functional materials developed in part at the Air Force Research Laboratory, Materials and Manufacturing Directorate. In collaboration with UES, Inc., Ohio University, and the ASC MSRC, a research program has been launched to understand the relationship between the structure of the foam and its mechanical and heat transfer properties. Pitch-based carbon foams are very rigid and highly thermally conductive, and thus are attractive for such applications as heat exchanger cores (which experience high acoustic loads) and spacecraft radiator panels (which can also act as structural components). With ever-higher performance, weight, and cost demands, multi-functionality is increasingly driving materials development.

Figure 1. Robo-Met.3D apparatus showing the polisher (left), robot arm (center) and optical microscope (right).

The background image shows a Robo-Met.3D rendering of a pitch-based carbon foam revealing the complex structure of its open-celled pores. Robo-Met.3D, invented by Spowart and Mullens, is a system to create three-dimensional reconstructions of complex material microstructures using automated metallographic serial sectioning and optical microscopy. Although originally designed to examine the microstructure of advanced metallic materials, the sectioning procedure is highly flexible, and the machine is equally adept at polishing metals, polymers, ceramics or composite specimens. The robot arm (Figure 1, center) cycles the sample between the polisher, (which removes a few microns from the surface), the rinse/dry station, and the automatic microscope.

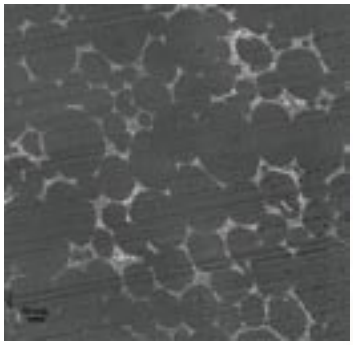


Figure 2. Optical Micrograph of Pitch-based Carbon foam. Light regions are foam, darker regions are epoxy filler.

Figure 2 is an optical micrograph of the foam and epoxy, which constitutes a single slice of the 3D image. After the images of successive slices are acquired, the software binarizes and reconstructs the microstructure using a custom visualization code based on Kitware's Visualization Toolkit (VTK). The 3D surface model can then be exported for finite element analysis of mechanical and thermal properties.

The need for HPC in this project is extensive. The surface model data sets are greater than 100MB (stl file format) for small models. The resultant solid models for finite element analysis are far too large for desktop systems. Scientific visualization in 3D is another need: Structures must be edited to remove unwanted features (for example, scratches from polishing that are interpreted as structure) or to correct polygonalization errors. Finding and correcting these in the highly complex foam structure is extremely difficult in two-dimensional viewers.

Finally, the structure of the pores, openings between pores, and node and ligament geometries are to be analyzed for size and shape dispersity, alignment, and microstructural anisotropy. For example, ellipsoids can be used to approximate pore sizes and shapes. Using the ASC MSRC's Scientific Visualization Laboratory's 3D viewing station, the quality of the ellipsoid approximation to the actual foam can be readily evaluated. The domain size and orientation of the graphitic carbon microstructure of the foams can be imaged by polarized light microscopy (see Figure 3), where the colored regions correspond to domains of different orientation. When this information is built into the 3D model, the texture and domain effects can also be accounted for in three dimensions.

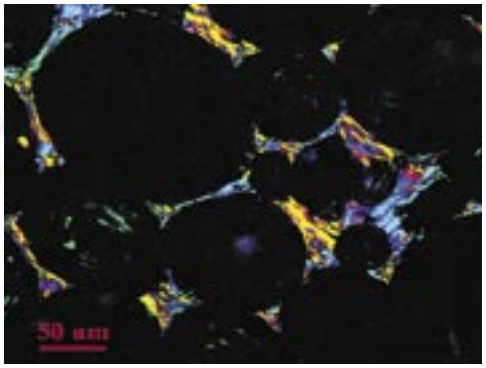


Figure 3. Polarized light microscopy image. Carbon birefringence gives rise to colors corresponding to microstructural domains.

In summary, this is a project in which HPC and scientific visualization will enable more realistic models of complex heterogeneous materials structures, and speed their transition to Air Force weapons systems.

This project represents a collaborative effort between: Benji Maruyama, Air Force Research Laboratory, Materials and Manufacturing Directorate; Jonathan E. Spowart, UES, Inc.; Daylond J. Hooper, Herb Mullens, Wright State University; Adriana M. Druma, Calin Druma, and M. Khairul Alam, Ohio University; and Rhonda Vickery, Darwin Adams, Chuck Abruzzino, and Terry McClurg, ASC/HPT.

HPC Breaking News

Introducing a New Activity in the HPCMP - Capability Applications Projects (CAP)

An exciting new opportunity for scientists and engineers in the DoD HPCMP was introduced this year – the Capability Applications Projects (CAP) activity. CAP provides a unique opportunity for scientists and engineers to test their application codes on a substantial portion of the new large systems, to perform leading-edge science and technology, and to solve large, meaningful problems in a relatively short time.

Several new single HPC systems, with over 2,000 processors and over two terabytes of memory, are now a part of the HPCMP. Before these new systems began operating under the HPCMP's standard allocation policy, a period of one to three months was dedicated to supporting the selected CAP activities.

The goals of CAP are to: 1) quantify the degree to which important application codes scale to thousands of processors, and 2) enable new science and technology by applying these codes in dedicated, high-end, capability environments.

In calendar year 2005, the ASC MSRC will become a firsthand player in the CAP activity when we receive our new large HPC system. We are looking forward to becoming an active participant in this new HPCMP endeavor.

HPCMPO Announces Open Research Systems

In the spirit of the National Policy on the Transfer of Scientific, Technical, and Engineering Information, National Security Decision Directive 189, and with the recognition that a significant portion of its computational workload falls under this policy that governs fundamental research, the HPCMPO is implementing an "open research systems" capability. Open research systems will require fewer user restrictions than normally required for access to DoD information systems. In particular, National Agency Check (NACs) will no longer be required for a valid DoD user to access open research systems, provided that the computational work done on these systems is unclassified with unlimited distribution. All other standard HPCMPO policies and procedures will remain active on open research systems.

Effective October 1, 2004 the Cray X-1 and the IBM P4 at the Arctic Region Supercomputing Center (ARSC) became open research systems. These systems are dedicated to supporting computational work where the results are specifically intended for public release, nominally in discipline-specific research programs such as conferences, proceedings, or technical journals. This implementation is being made to provide more timely access to the HPCMPO computing resources for a large, important segment of our user community, yet still maintaining the access restraints imperative on sensitive but unclassified systems.

Users with computational work that does not have unlimited distribution will not be allowed to use open research systems and will continue to access other HPCMPO HPC systems that will continue to require trustworthiness certification.

For more information contact ARSC via email at *info@arsc.edu*.

High-End Computing Revitalization Task Force Findings

The following information was taken from the Report of the High-End Computing Revitalization Task Force, dated May 10, 2004. The complete report is available at www.itrd.gov/pubs/2004_hecrtf.

In 2003, the DoD, DOE, and the National Science Foundation (NSF) initiated independent planning activities to address technology and resource issues. After examining these activities, the Office of Science and Technology Policy (OSTP) determined that an effort focused on high-end computing (HEC) was warranted. The High-End Computing Revitalization Task Force (HECRTF) was chartered under the National Science and Technology Council (NSTC) to develop a plan for undertaking and sustaining a robust Federal high-end computing program

to maintain U.S. leadership in science and technology.

As stated in the final report referenced above, “The overarching conclusion of the Task Force is that action to revitalize high-end computing in the U.S. is needed now.” The Federal government’s historical success in motivating HEC R&D, the oversubscription of current HEC resources, the scarcity of alternative architectures for delivering high performance to applications, and the lack of current incentives for industry to engage in HEC architecture research all argue strongly that the Federal government should move to revitalize HEC R&D.

The Task Force outlined several steps toward the goal of a healthy and vibrant high-end computing environment:
Key research and development application areas and user requirements that guide directions for establishing roadmaps and investments in hardware, software, and systems technologies were identified. Gaps in accessibility of Federal agencies to HEC capabilities to meet agency missions were also identified.

The Task Force presented a more effective approach to HEC procurement. Additionally, the establishment of an Interagency Program Office to manage and integrate the technology, resource, and procurement process to assure efficient and effective HEC investments and results across government agencies was discussed.

As stated in the final report delivered by the Task Force, “The U.S. government must re-establish its role as the key proponent of HEC systems for the nation’s scientific and engineering research and development.”

FY05 Challenge Projects Announced

On August 12, 2004, the HPCMPO announced the selection of 15 new Challenge Projects, while also authorizing the continuation of 21 previously selected multi-year Challenge Projects for FY05.

Selection of new Challenge Projects occurs annually through a rigorous technical and mission relevance evaluation. These projects are deemed to be computationally intensive and of high priority. Twelve of these 36 projects will run at the ASC MSRC during FY05.

Returning from FY04

- 3-D CFD Modeling of the Chemical Oxygen-Iodine Laser II - Air Force
- Computational Simulations of Combustion Chamber Dynamics and Hypergolic Gel Propellant Chemistry for Selectable Thrust Engines in Next Generation Guided Missiles - Air Force
- Defense Against Chemical Warfare Agents (CWAs) and Toxic Industrial Chemicals (TICs): Filtration, Prophylaxis and Therapeutics - Army
- Multidisciplinary Applications of Detached-Eddy Simulation to Separated Flows at High Reynolds Numbers - Air Force Academy
- Three-Dimensional Modeling and Simulation of Weapons Effects for Obstacle Clearance - Navy
- Time Accurate Unsteady Simulation of the Stall Inception Process in the Compression System of a US Army Helicopter Gas Turbine Engine - Army
- Tip-to-Tail Turbulent Scramjet Flowpath Simulation with MHD Energy Bypass - Air Force

New in FY05

- Applications of Time-Accurate CFD in Order to Account for Blade-Row Interactions and Distortion Transfer in the Design of High Performance Military Fans and Compressors - Air Force
- Virtual Prototyping of Directed Energy Weapons - Air Force
- Simulation of a Dynamically Maneuvering Unmanned Combat Air Vehicle - Air Force
- Millimeter-Wave Radar Signature Prediction Improvement for Ground Vehicles - Army
- Computer Design and Simulation of Molecular Devices and Energy Sources for Naval Applications - Navy

Hails and Farewells

Steve Baxter, CSC Business Office manager, transferred to Raleigh, North Carolina, to support a CSC contract.

Katherine Rath, OSC, was named PET Component 2 Program Assistant in July.

Jason Boudi, ASC/ HPTT, joined the ASC MSRC in September.

Ryan Cappo, CACI, joined the ASC MSRC team in July.

Randy Pargman, CACI, left the ASC MSRC for a position with the FBI in August.

Pam McCarty, CSC, was named Program Control Officer in September.

Nick Pelligrini, CSC Integration Specialist, transferred to Raleigh, North Carolina, to support a CSC contract.

Sharron Madero, of the PET team, remains with OSC at their Springfield Technology Park office.

Dinah Luneke, CSC, joined the ASC MSRC team in October.

Gary Meyer, CSC, Applications Manager, retired in July.

Tony DelSorbo, CSC, moved to the Advanced Technologies group in July.

Jay Blair, CSC, moved to the Advanced Technologies group in July.

Gary Sivak, ASC/HPTA, was promoted to GS-13.

Tim Yeager, CSC, was named manager of the database and web teams in September.

Tracey Smith, CSC, was named Computational Technology Center manager in July.

GS-320 was acquired by AFRL/ML.

Tim Sell, ASC/HPTA, joined the ASC MSRC in July.

IBM P3 was decommissioned in October.

Dave Potts, ASC/HPTT, retired after 30 years of Government service.

Staff Support a Variety of Conferences

By Maria Zimmer, ASC/HPTA

In order to keep pace with the ever changing HPC landscape, management and staff of the ASC MSRC support various conferences throughout the year. Below are descriptions of some of these conferences.

The DARPA High Productivity Computing Systems (HPCS) conference held in Fairfax, Virginia June 2004, was attended by Steve Wourms, the ASC MSRC Director and Bill Asbury, CSC Deputy Program Manager. One of the goals of the HPCS is to create an acquisition framework for HPC that addresses productivity as a result of execution and development time.

The First Annual HPC Users Conference was held in Washington, D.C. July 12-13, 2004. Steve Wourms and Bill Asbury attended this conference. Sponsored by the Council on Competitiveness, this conference has a three year initiative: To galvanize a dialogue among government agencies, industry manufactures and private sector users of HPC to leverage government investment in HPC research and development for a more vibrant, dual-use market.

Symposium on the Use of Commodity Clusters for Large-Scale Scientific Applications was held in Tysons Corner, Virginia, July 26-29, 2004. Attending from the ASC MSRC were Jeff Graham, Deputy Director; Donna Klecka, CSC Program Manager; Tony DelSorbo, CSC Advanced Technologies; and Phil Amburn, PET FMS on-site lead. This symposium focused on technology trends, production/performance issues, tools, networking and storage, and applications.

SIGGRAPH 2004 was held August 8-12, 2004 in Los Angeles, California. Brian Schafer, ASC/HPTT; Chuck Abruzzino, CSC; and Rhonda Vickery, PET ET on-site lead, previewed future trends in data analysis and visualization at this annual conference. Conference papers and short courses described progress made in areas such as computer graphics, high resolution and 3D displays, rendering and dynamic modeling. Exhibitors demonstrated new tools and advances in 3D visualization, rendering and shading, and graphics processors. The information gathered will be used to better meet the data analysis and visualization needs of ASC MSRC customers.

2004 Monterey Grid Computer Conference was August 9-12, 2004 in Monterey, California. Jay Blair, CSC, presented ASC's work on Visual Queue and Batch Engine at this conference sponsored by the Fleet Numerical Meteorology and Oceanography Center (FNMOC).

A list of upcoming conferences is shown on the following page. If you would like to learn more about the ASC MSRC presence at these conferences or are interested in other Outreach activities, please contact us via email at *asc.hp.outreach@wpafb.af.mil*.

Upcoming Conferences

November 6 - 12, 2004
Supercomputing Conference 2004
David L. Lawrence Convention Center
Pittsburgh, Pennsylvania
www.erdc.hpc.mil/SC04/SC04.htm

November 29 - December 2, 2004
24th Army Science Conference
JW Marriott Orlando Grande Lakes
Orlando, Florida
www.asc2004.com

November 29 - December 3, 2004
Materials Research Society (MRS) Fall Meeting
Hynes Convention Center
Boston, Massachusetts
www.mrs.org/meetings/fall2004

December 6 - 9, 2004
I/ITSEC
Orange County Convention Center
Orlando, Florida
www.iitsec.org

December 13 - 16, 2004
ITEA Modeling and Simulation Workshop
Hilton Hotel
Las Cruces, New Mexico
www.itea.org

January 10 - 13, 2005
43rd AIAA Aerospace Sciences Meeting and Exhibit
Reno Hotel
Reno, Nevada
www.aiaa.org

June 27 - 30, 2005
DoD Users Group Conference
Gaylord Opryland Resort and Convention Center
Nashville, Tennessee
www.hpcmo.hpc.mil/Htdocs/UGC

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